1-[«alpha»-Methoxycarbonyl(phenylmethyl)]-2-me

Inchi: InChI=1S/C10H12N2O4/c1-15-10(13)9(12(14)11-16-2)8-6-4-3-5-7-8/h3-7,9H,1-2H3
InchiKey: UFZBWIWHYPNSLN-UHFFFAOYSA-N
Formula: C10H12N2O4
SMILES: CON=[N+]([O-])C(C(=O)OC)c1ccccc1
Mol. weight [g/mol]: 224.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	1.425		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
rinpol	1691.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121465&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices